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# Using Databases to Streamline Process Design and Analysis

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**Abstract**

The design and analysis of chemical processes can be performed using countless methods from rigorous computer simulation to simple spreadsheet calculations. However, all methods require significant process design and cost data to ensure valid, reproducible results. Obtaining this information can represent a substantial amount of effort for the process engineer. Often, the collection and inputting of data is repeated over and over for each new design because the data cannot be easily transferred between design applications or because documentation is lost. To streamline the use of process data, NREL engineers utilize databases to store equipment designs and costs as well as operating costs and documentation. Information from the databases is then electronically linked with spreadsheets where it is combined with mass and energy balance information from a linked process simulation package (ASPEN+) to generate economic analysis data such as capital investment and production costs. When process stream flows do not vary drastically, scaling factors are used to provide new costs based on the process's stream information. There are several advantages to this system. Information resides in one place, eliminating dual or conflicting data, and can be linked to many process designs. When a change is made, all users of the information have it at the same time. As the knowledge base grows through additional data, the information can be compared, averaged and manipulated to reduce the range of error in economic analyses.

Keywords: database, process design, economic analysis, spreadsheet

Process design is an exercise in compiling virtual data and using it to develop a set of specifications that will be used to build a real plant. Because the time frame from conception to construction is usually on the order of several years, information can become lost, obsolete, or its origin uncertain. In order to complete the exercise with the least amount of rework, it is crucial that all data be captured and documented as completely as possible as it is incorporated into the process specifications.

Databases, a relatively new tool in the computing arsenal available on personal computers or networks, can be invaluable in the endeavor to move process designs forward efficiently.

Research at the National Renewable Energy Laboratory (NREL) focuses on discovering ways to produce energy from sources that are virtually limitless or can be replenished using known methods. Wind and sun are examples of virtually limitless sources that can be used to produce power; crops such as wood, grasses or waste can be replenished and can provide power, fuels for power, and chemicals. The fuels development work at NREL focuses on producing alcohol, aromatics, and diesel products as fuels or blending agents for gasoline from biomass or wastes. The process, like any, is made up of several steps. Some of the processing steps are novel and particular to biomass such as hydrolysis (breaking up the biomass into useable compounds). Others, like alcohol distillation, are well understood developed due to widespread use in the chemical processing industries. Another challenge routinely encountered is using an established process, such as evaporation or anaerobic digestion of wastewater, on a new set of components.

Process engineering work in the Biotechnology Center for Fuels and Chemicals at NREL focuses on providing information to research staff, outside companies, and DOE program managers to help them determine what research programs will be most effective at improving the costs of fuel production from biomass. Our approach to process design and economic evaluation is comprised of four stages or pieces, shown in Figure 1.

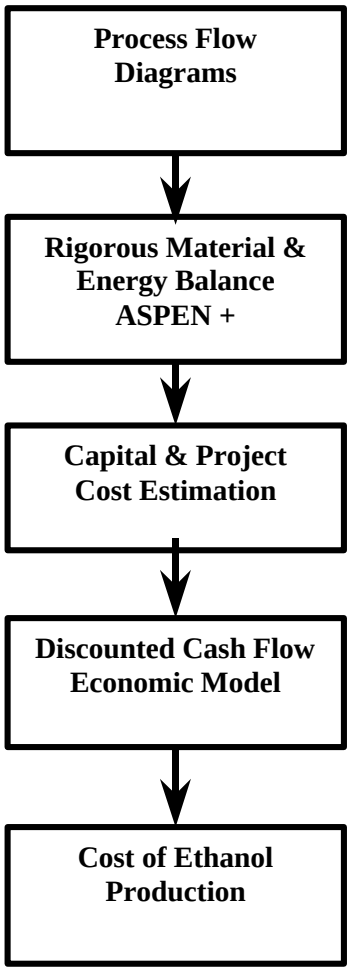


**Figure 1**
**NREL's Approach to Process Design and Economic Modeling**

Information from many sources is used to develop the process flow diagrams, build a rigorous model of the process in ASPEN+, and compile a capital and project cost estimation. Figure 2 shows examples of the information sources typically used. When industry proven designs and

costs are available, such as from engineering construction (E/C) firms or vendors, they are used. NREL has used subcontracts to work with E/C firms on the design of several ancillary systems, and similar subcontracts with research institutions to add to NREL's in-house research effort. Cost estimation software is used when vendor information is not available.

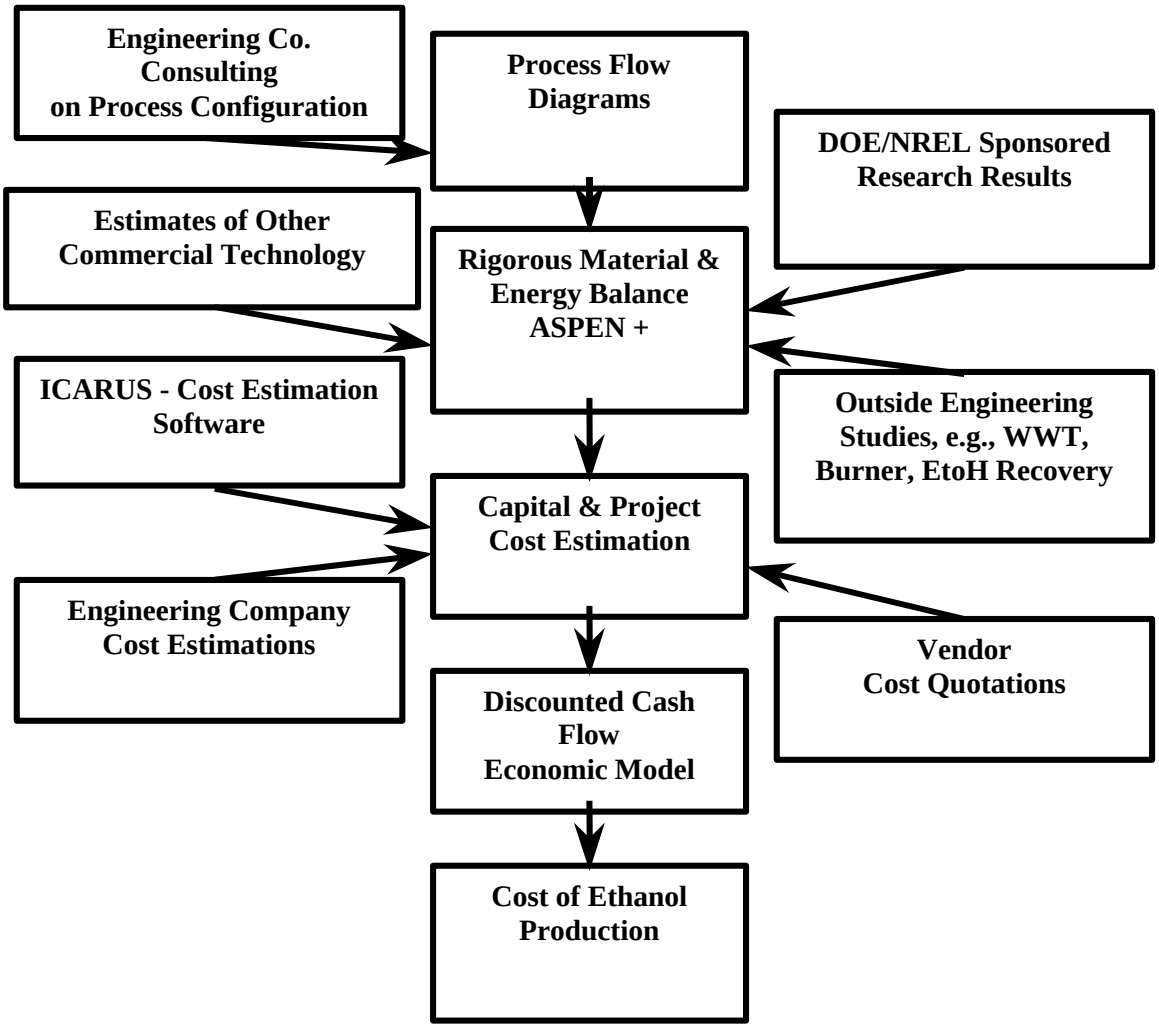


**Figure 2**
**Sources of Information for NREL model**

As a process engineer involved with the design, modeling and economic analysis of biomass processes, I experienced the time-consuming tasks of finding data, inputting it, documenting it,

then doing it all over again for a new process or process modification. To reduce the time required to get and use data to develop processes, and to avoid losing data over the long project, the Process Engineering team at NREL developed three databases to store information ranging from feedstock composition, equipment specifications and costs, and completed process models. Graphical User Interfaces (GUI) were designed by the engineers to access the databases, either to put in information or take it out. These databases are also linked to our spreadsheets that generate capital and production cost summaries. Data from the databases feeds into the spreadsheets through electronic links, which eliminates manual data entry.

Populating the databases originally represents a large time commitment, but administrative assistants have done the bulk of it. Portable Document Format (pdf) files are used for hard copy quotes and specifications so that supporting documentation is not separated from the data. Scanning vendor quotes into pdfs, entering data into fields on a GUI, and adding electronic files with design specifications are all easy to do. Figure 3 shows an example of the GUI we use to enter equipment specification and cost data. Scaling and installation factors and pertinent data about process streams that the equipment is design for can also be added to the equipment record.

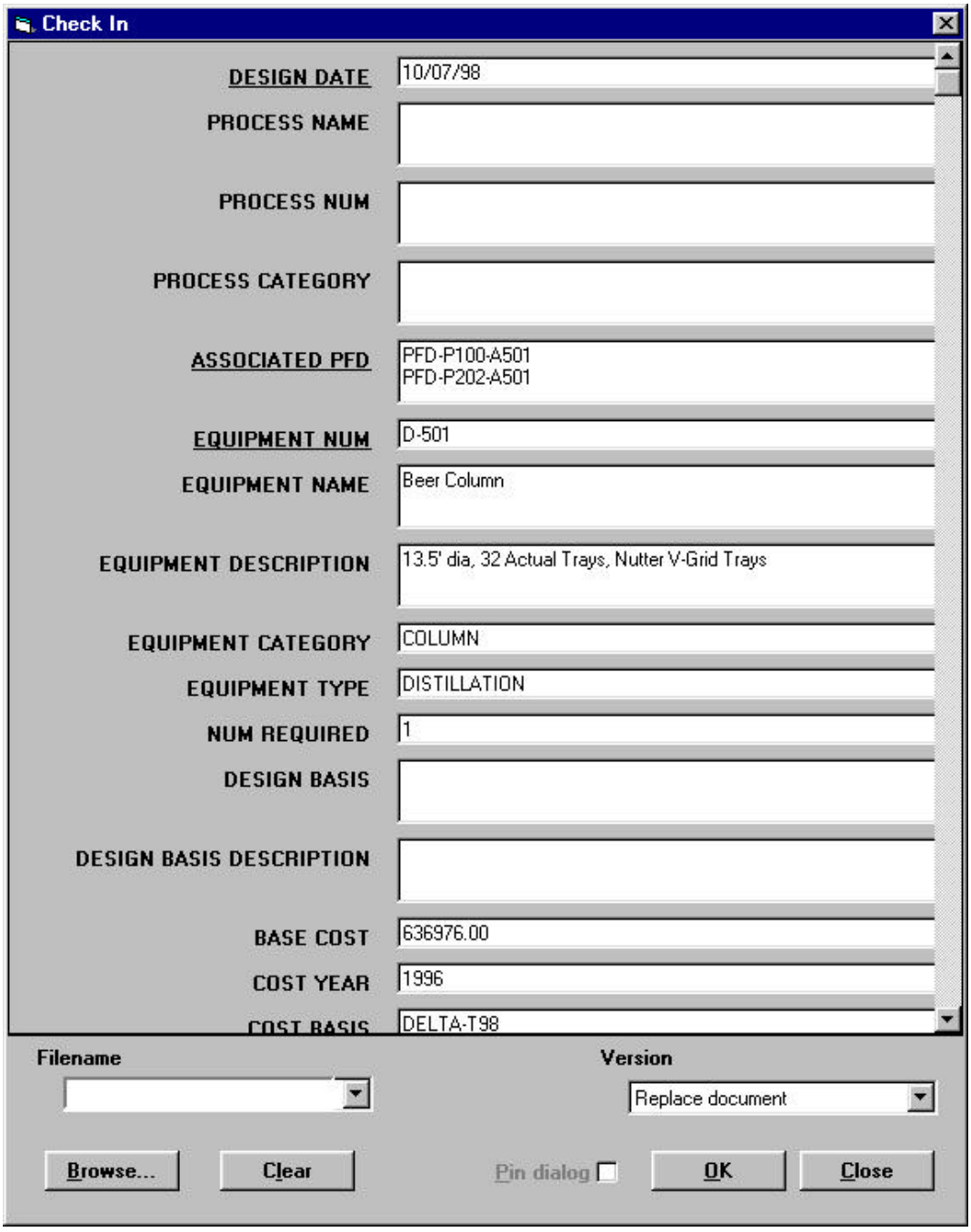


**Figure 3**
**Equipment Database Input Screen**

Figure 4 shows Feedstock database GUI, developed in Visual Basic. The feedstock database stores information on a range of biomass types including composition and physical properties. This data is used in modeling and is added any time that analytical work is done, so the database grows and becomes more robust.

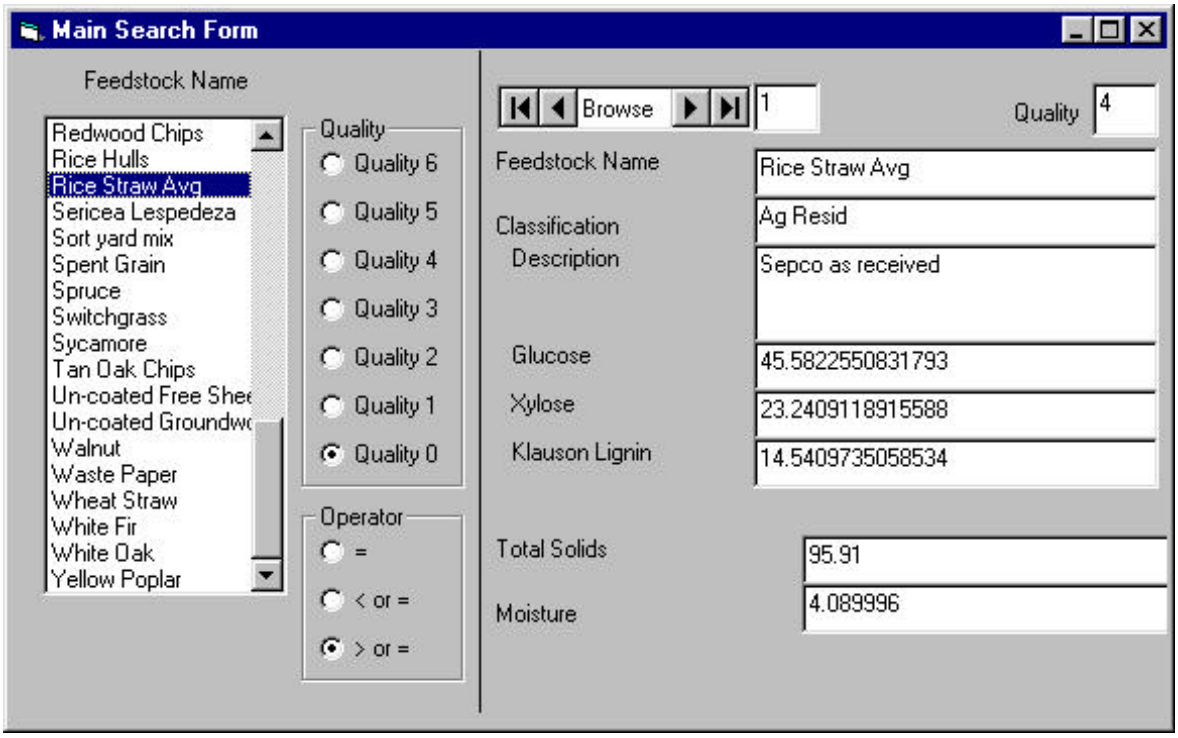


**Figure 4**
**Biomass Feedstocks Database Search Screen**

Figure 5 shows the links between databases and process design tools, namely AutoCAD drawing files, ASPEN+ models and Excel spreadsheets and also the links between ASPEN+ and Excel. Retrieving data can be done manually or through an electronic link that can be updated automatically or when a specific event occurs, such as when the file is opened. An example of manual retrieval would be taking physical property data from the feedstock database to enter into ASPEN+ or for a researcher to use in designing an experiment. Electronic retrieval is used to transfer capital and operating costs from the database into the economic analysis spreadsheet. A query is a request for information from a database. Many software applications now have built in query wizards that help you find the database, determine what you want out of it and how you want it sorted.

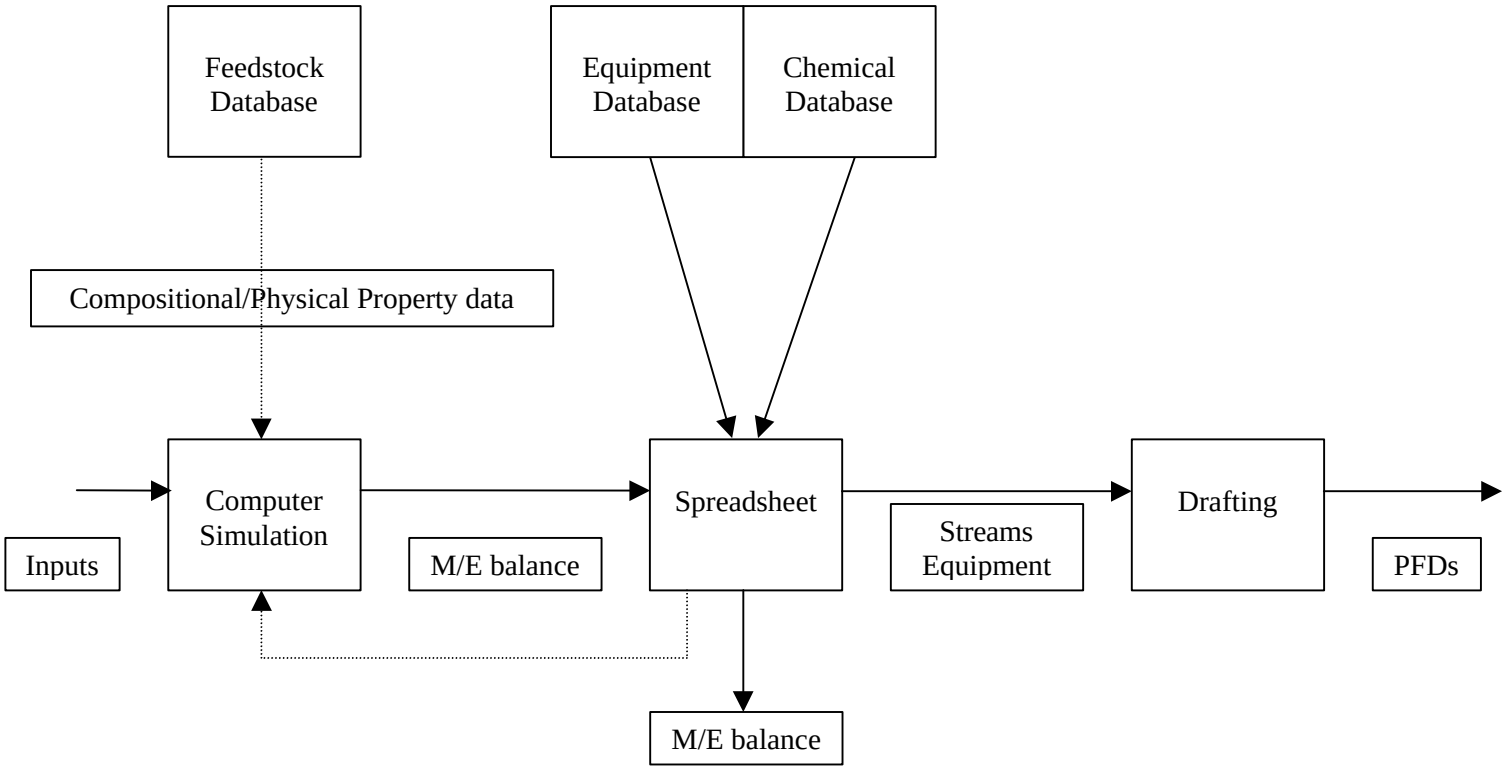


**Figure 5**
**Linkages**

Figure 6 shows the Query Wizard from Excel, for example. Data is dumped to a worksheet in the workbook.

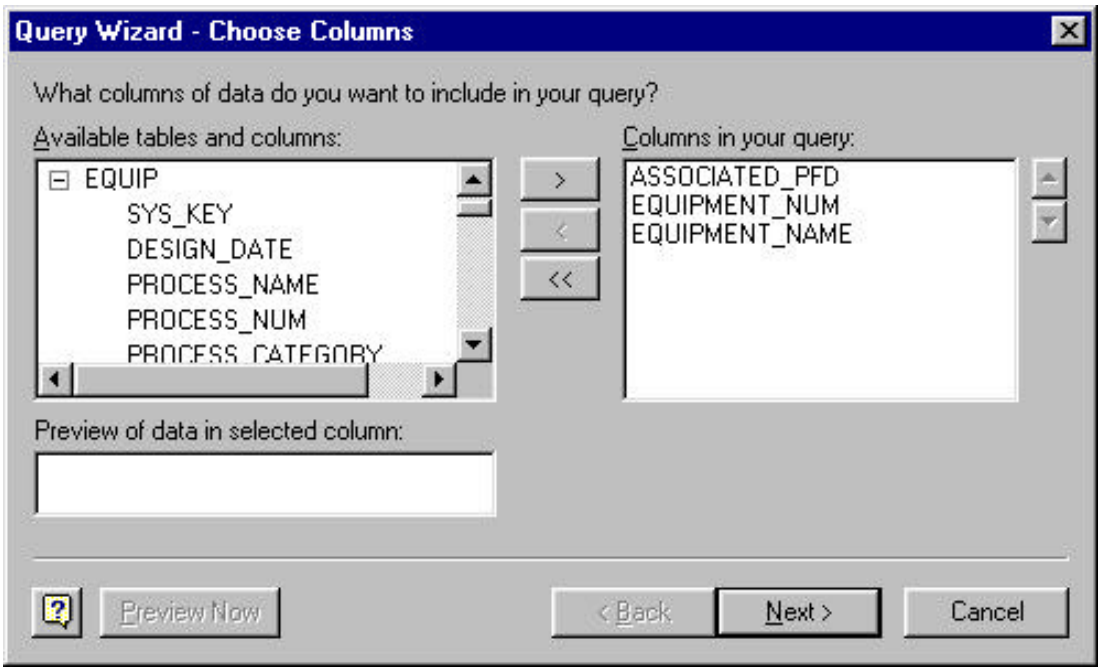


**Figure 6**
**Excel Query Wizard**

The data can be refreshed, or re-retrieved easily. For most process designs, we do not refresh data unless there has been significant changes to the equipment specs that we want to capture. From this worksheet, using either links or a lookup function, you can add the data to any worksheet. For example, we use separate sheets to tabulate capital and operating costs. This method works particularly well for us because we scale equipment from one base cost per item to a new cost using flow, area, or other process parameters. The advantage is that you can produce several different versions of a process (plant size, yield, and even specific reaction parameters such as temperature or residence time) quickly. For a more rigorous design, such as an engineering construction firm might employ, the cost database might have different quotes for different sizes of one piece of equipment. Equipment specifications can be linked to drawing files to avoid time-consuming drafting changes. Data from the ASPEN+ model, downloaded into the spreadsheet to scale the costs, can also be dynamically linked to a drawing to provide process specs on the drawing.

Once a process design has been completed, the ASPEN+ model, economic spreadsheet, and process drawings are stored in a third database, a repository of models. These files can be retrieved and reviewed, referenced in reports or used as building blocks for a new design. Figure 7 shows the GUI for the models database. Having previous models available for all process engineers, along with documentation about what the model does, is invaluable in modeling new processes quickly.

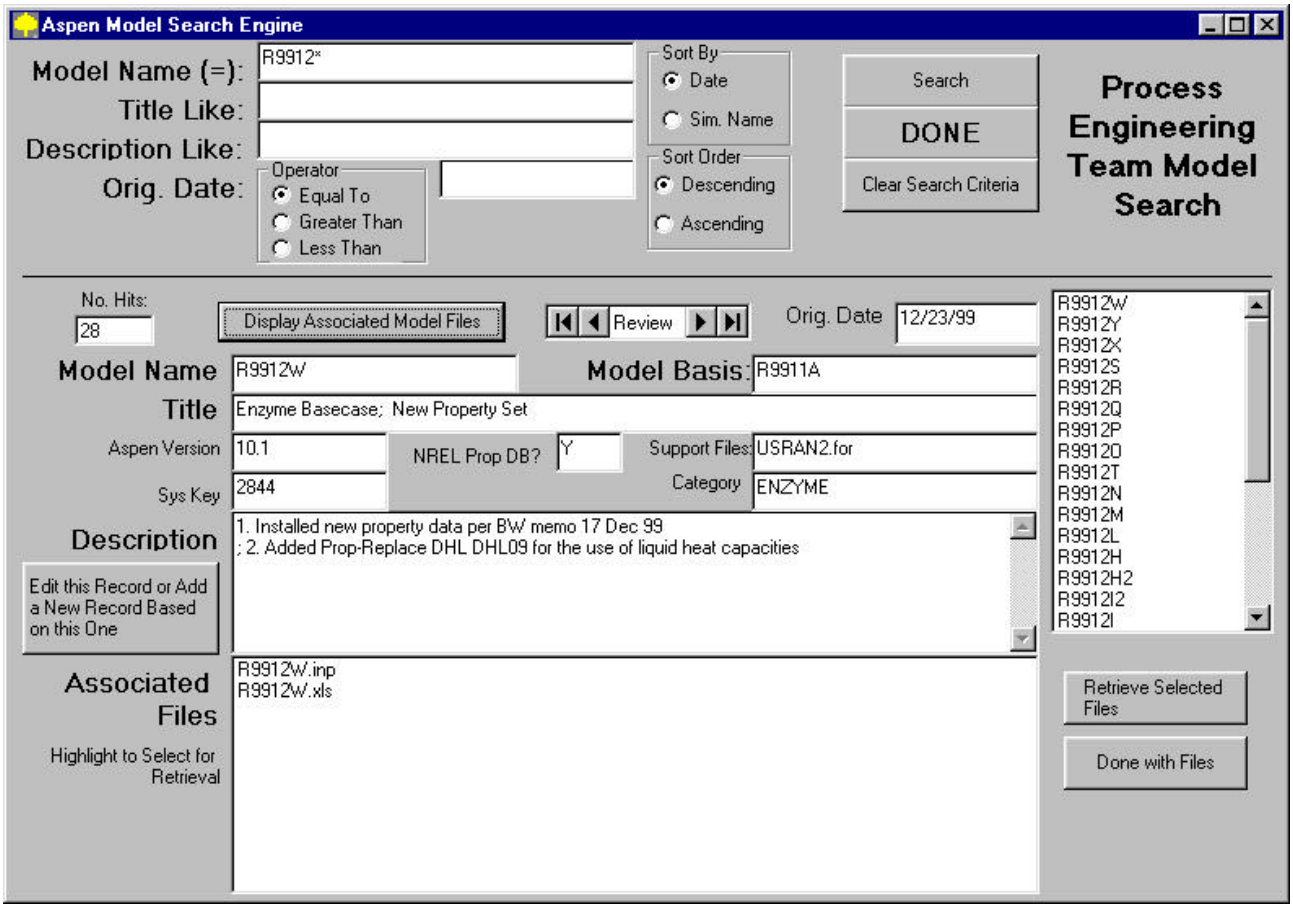


**Figure 7**
**Repository for completed models**

There are several advantages to using databases and linkages to them for process design:

1) Every engineer uses the same data for the same equipment specification, eliminating dual or conflicting information.
2) Only one change is needed to update an unlimited number of process designs.
3) We are building a repository of information that can be compared, averaged, and manipulated to reduce the range of error in our economic analyses.
4) Making good use of scanning, vendor quotes and other supporting documentation is added to the database in .pdf format, making it easy to access crucial documentation and keep organized and updated.

5) Complete databases of information can be burned onto a CD for easy transfer to customers, contractors, and suppliers.

In research, poor funding decisions can result in lost money and time pursuing the wrong path. Building a storehouse of data and using it consistently in all process designs can help improve the odds in decision making by providing objective, supported analyses.

# Using Databases to Streamline Process Design and Analysis

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## Renewable Energy From:

- Wind (turbines)
- Sun (photovoltaics)
- Biomass (trees, grasses, residues)
  - Power
  - Fuels
  - Chemicals

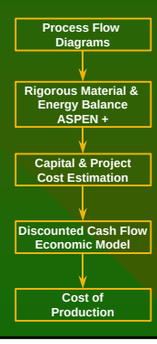
## Fuels like…

- Ethanol
- Aromatics
- Biodiesel

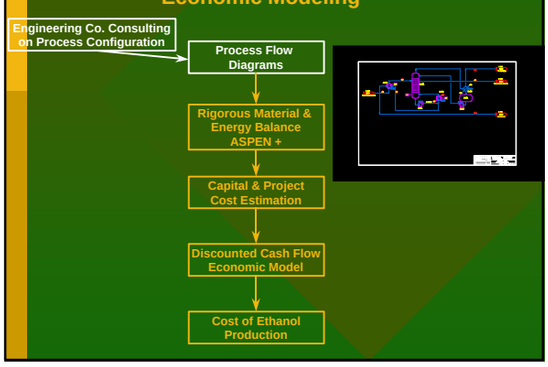
## Processes like...

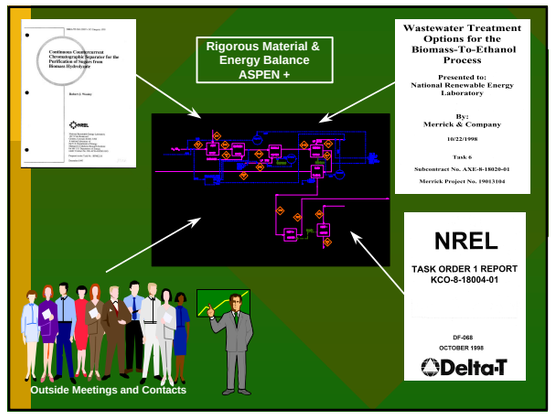
- Solids Handling
- Fermentation
- Distillation
- Evaporation
- Digestion
- Combustion

## NREL's Approach to Process Design and Economic Modeling




## NREL's Approach to Process Design and Economic Modeling



## Capital & Project Cost Estimation

| Equip Name | Original Equip Cost (per unit) | Base Year | Scaling Exponent | Installation Factor | Installed Cost in 1997$ |
|---|---|---|---|---|---|
| Hopper Feeder | $8,000 | 1999 | 0.76 | 1.3 | $40,679 |
| Transfer Belt Conveyor | $78,000 | 1999 | 0.76 | 1.3 | $99,307 |
| Radial Stacker Conveyor | $200,100 | 1999 | 0.76 | 1.3 | $254,369 |
| Reclaim Hopper Feeder | $8,000 | 1999 | 0.76 | 1.3 | $20,339 |
| Reclaim Hopper Conveyor | $172,976 | 1997 | 0.76 | 1.3 | $219,889 |
| Chip Washer Feeder | $5,500 | 1999 | 0.76 | 1.3 | $27,967 |
| Scalper Screen Feeder | $13,392 | 1998 | 0.76 | 1.3 | $34,429 |

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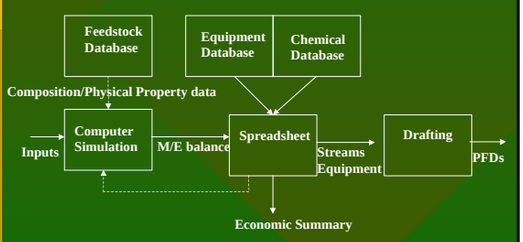
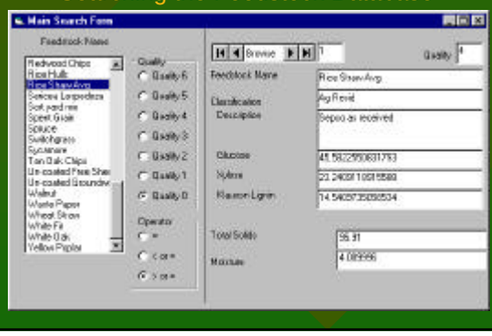
## How to Keep Track of it All?

- Developed 3 databases (1 in UNIX, 2 in MS ACCESS)
- Developed 3 Graphical User Interfaces (GUI) to access databases (Visual Basic)
  - Compositional data on Feeds (FEEDSTOCK)
  - Capital & Operating Costs (EQUIPMENT)
  - Complete models (REPOSITORY)

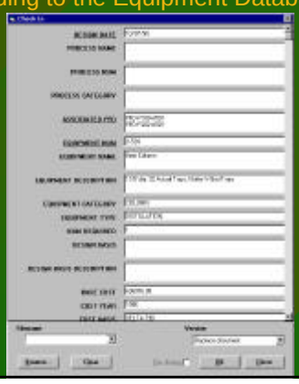
## Linkages Between Databases and NREL Model Components




## Searching the Feedstock Database




## Adding to the Equipment Database



## Everything into one Place

### WITH CONCENSUS

Major Aspects of Database

Equipment ID
Equipment Name
Equipment Description/Size
Number of Pieces
Number of Spares
Scaling Size
Base Cost
Source of Cost
Scaling Exponent
Source of Scaling Exponent
Installation Factor
Source of Installation Factor
Material of Construction

NREL Engineers Using ASPEN, Spreadsheets, Other Methods

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## Other Important Information in Equipment Database

- Variable Operating Costs
- Scaling Item from Aspen
  - Identification of Item
    - Flow, Duty, Area
  - Base Value
  - Units
- Information Sources (pull-down menus)

## ASPEN Plus Simulation Information Transferred to Excel

| Variable Name | Value | Units |
|---|---|---|
| AREA0302 | 3,700 | |
| DIAMD501 | 3.89 | METER |
| INUMSSFA | 34 | |
| QRFD0502 | 986,470 | CAL/SEC |
| STRM0502 | 380,206 | KG/HR |
| WRKWTOTL | -41,651 | KW |
| Total Number of Items Retrieved: 154 | | |

Calculated in FORTRAN in ASPEN

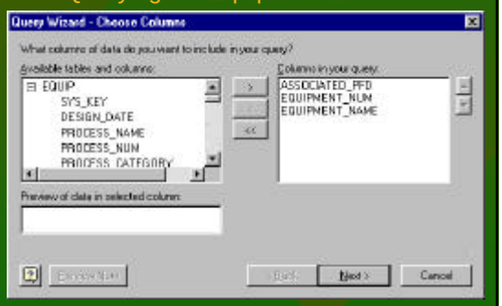
Unit Operation Variable

Heat Stream Duty

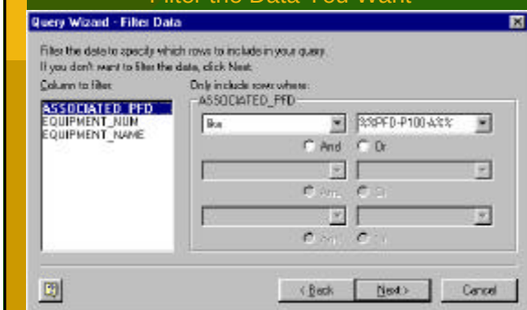
Material Stream Flow

Work Stream Power

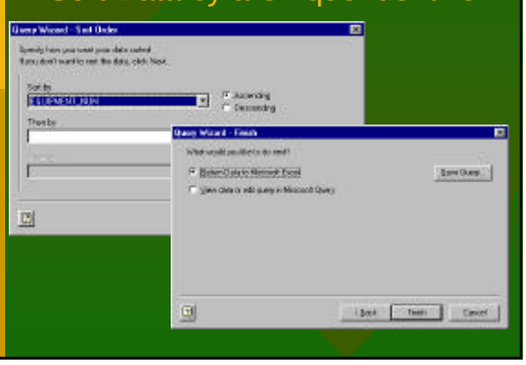
## Querying the Equipment Database



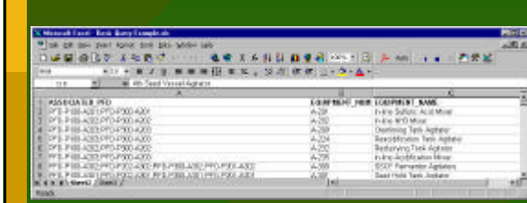

## Filter the Data You Want




## Sort Data by a Unique Identifier




## Add the Data to Excel Workbook



## Link Data to Worksheets

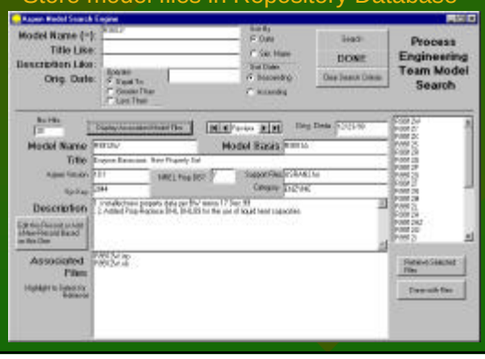
| EQUIP NUM | Equipment Name | NUM REQ. | BASE FOR SCALING | BASE COST | SCALE EXP |
|---|---|---|---|---|---|
| A-300 | SSCF Fermentor Agitators | | | 19676 | |
| A-301 | Seed Hold Tank Agitator | 1 | 41777 | 12551 | 0.51 |
| A-304 | Seed Fermentor Agitators | 2 | 41777 | 11700 | 0.51 |

## Equipment Cost Scaling in Excel

| Equip No. | No. Req'd | No. Req. Variable | Scaling Item | Scaling Item Value | New Item Value | Original Equip Cost (per unit) | Total Equip Cost | Scaling Exp. | Scaled Cost |
|---|---|---|---|---|---|---|---|---|---|
| A-300 | 34 | INUMSSFA | | | | $ 19,676 | $ 668,984 | | $ 668,984 |
| A-301 | 1 | | STRM0304 | 41,777 | 37,997 | $ 12,551 | $ 12,551 | 0.51 | $ 11,958 |
| A-304 | 2 | | STRM0304 | 41,777 | 37,997 | $ 11,700 | $ 23,400 | 0.51 | $ 22,295 |

**Hard-coded into spreadsheet**
**ASPEN PLUS Value - Look-up From ASPEN Plus Link**
**MS Access Database Value - Look-up from MS Access Link**
**Calculated Value**

## Store model files in Repository Database



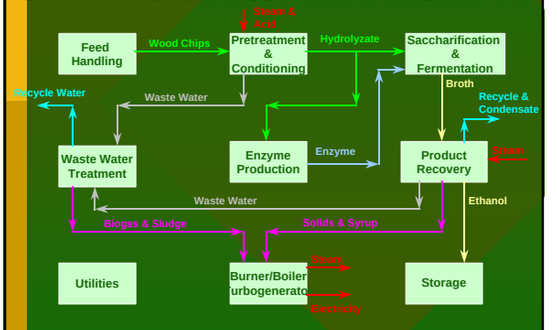

## Advantages to Using Databases

- Allows data collection/averaging
- Achieves consistency in costing processes
- Allows rapid, consistent comparison of different process designs
- One change in database changes spreadsheets
- Repository for models that can be referenced
- Source and quality of data is verifiable

## For more information:

- About Database uses
  - Kelly_Ibsen@NREL.gov
- About Bioconversion for Fuels and Chemicals
  - www.Biofuels.org
  - www.NREL.org

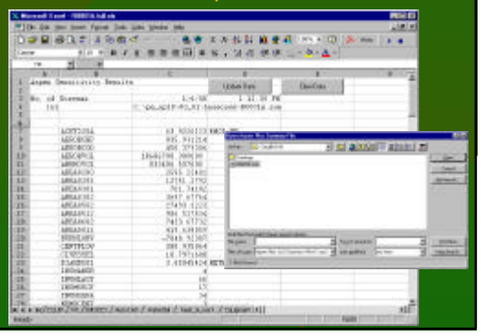
## Bioethanol Production via Dilute Acid Pretreatment & SSCF



## Extract Information from ASPEN Plus

- Consolidate in Sensitivity Block
- Extract to Excel Look-up Table
  - From GUI Use Paste-Link
  - From Input File Mode Use VB-Summary File Tool Kit

## Import Mass/Energy information from Aspen+



## Approach to Detailed Process Modeling

- **Use Detailed Modeling to Support and Interpret Experimental Work**
  - **Fortran, MatLab, Aspen/Plus, Aspen/SP, Scientist, Excel, Others**
- **Translate Experimental Work and Detailed Modeling into "Simpler" Forms**
- **Use a Less Detailed ASPEN Model to Describe the Entire Integrated Process**